Aspects and prospects of KAERI atomic data center

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4-6 Sept. 2017, IAEA Headquarters, Vienna, Austria
Outline

2. KAERI Atomic Database Updates
3. Summary and Outlook
Research Activities

1. **State-of-the-art calculations** for the **electron-impact ionization** and recombination, and **photoionization data** which are essential in modeling for laboratory and astrophysical plasmas.

2. **Spectroscopic measurement** in plasma devices and **collisional radiative modeling** for analysis on the measured spectra.
1. Dielectronic recombination (DR)
   - Highly charged $W^{44+} \sim W^{46+}$
   - Lowly charged $W^{5+} \sim W^{11+}$

2. Photon emissivity coefficient (PEC)
   - $W^{5+} \sim W^{48+}$

3. Spectroscopic measurement & collisional-radiative (CR) modeling
   - Ar
Spectroscopic Modeling

Emissivity $\varepsilon_{ij}$ for line transition $i \rightarrow j$

$$\varepsilon_{ij} = n_Z(r,t)n_e(r,t)\text{PEC}_{ij}(T_e,n_e)$$

Photon Emissivity Coefficient

Charge $Z$ ion density from transport modeling

Electron density

Collisional excitation (CE) rate

Radiative transition probability

Simple coronal Model for state population density

$\sum_{k<i} X_{0i} A_{ik}$

$$\text{PEC}_{ij}(T_e) = X_{0i} \sum_{k<i} A_{ik}$$

Ground state for any charge state of $Z$ ions

Radiative transitions

Any $k$ below $i$

CE from 0 to $i$

$$n_e [\text{cm}^{-3}] \leq 5.6 \times 10^8 (Z + 1) \times 1.106 \times 10^{10} (Z + 1)^2 \exp \left[ \frac{1.162 \times 10^3 (Z + 1)^2}{T_e} \right]$$

with hydrogenic approximation

Atomic Data

$T_e [\text{eV}]^{1/2} \exp \left[ \frac{1.162 \times 10^3 (Z + 1)^2}{T_e} \right]$
Transport equation for charge Z ion

\[
\frac{\partial n_Z(r,t)}{\partial t} = -\nabla \cdot \Gamma_Z(r,t) + S_Z(r,t)
\]

**Transport term**

\[
\Gamma_Z(r,t) = -D(r) \frac{\partial n_Z(r,t)}{\partial r} + V(r) n_Z(r,t)
\]

**Diffusion coefficient**  **Drift, convection coefficient**

**Source & sink term**

\[
S_Z(r,t) = -n_e \left( \alpha_I^Z + \alpha_R^Z \right) n_Z + n_e \alpha_I^{Z-1} n_{Z-1} + n_e \alpha_R^{Z+1} n_{Z+1}
\]

**Ionization rate coefficient**  **Recombination coefficient**

**Atomic Data**
Photon Emissivity Coefficient (PEC)

$W^{q+} \ (q=5) \ ground \ state \ 4d^{10} \ 4f^{14} \ 5s^2 \ 5p^6 \ 5d, \ IE : 66.37 \ eV$

$4d^{10} \ 4f^{14} \ [5s^2 \ 5p^6 \ 5d]^{-1} \ n'l' \rightarrow 4d^{10} \ 4f^{14} \ [5s^2 \ 5p^6 \ 5d]^{-1} \ nl + h\nu$

$4d^{10} \ 4f^{13} \ 5s^2 \ 5p^6 \ 5d \ n'l' \rightarrow 4d^{10} \ 4f^{13} \ 5s^2 \ 5p^6 \ 5d \ nl + h\nu$

$\rightarrow 4d^{10} \ 4f^{14} \ 5s^2 \ 5p^6 \ 5d \ + h\nu \quad (n'=5,6, \quad n \leq n')$

$W^{q+} \ (q=6-11) \ ground \ state \ 4d^{10} \ 4f^{26-q-m} \ 5s^2 \ 5p^m \ (m=6-2), \ IE : 125.7 \ eV-234.2 \ eV$

$4d^{10} \ 4f^{26-q-m} \ [5s^2 \ 5p^m]^{-1} \ n'l' \rightarrow 4d^{10} \ 4f^{26-q-m} \ [5s^2 \ 5p^m]^{-1} \ nl + h\nu$

$\rightarrow 4d^{10} \ 4f^{26-q-m+1} \ [5s^2 \ 5p^m]^{-1} + h\nu$

$\rightarrow 4d^{10} \ 4f^{26-q-m+1} \ [5s^2 \ 5p^m]^{-2} \ n'l' + h\nu$

$4d^{10} \ 4f^{26-q-m-1} \ 5s^25p^m \ n'l' \rightarrow 4d^{10} \ 4f^{26-q-m-1} \ 5s^25p^m \ nl + h\nu$

$\rightarrow 4d^{10} \ 4f^{28-q-m} \ 5s^25p^m + h\nu \quad (n'=5,6, \quad n \leq n')$

$W^{q+} \ (q=12-16) \ ground \ state \ 4d^{10} \ 4f^{28-q-m} \ 5s^m \ (m=1 \ or \ 2), \ IE : 273.6 \ eV-390.2 \ eV$

$4d^{10} \ 4f^{28-q-m} \ 5s^{m-1} \ n'l' \rightarrow 4d^{10} \ 4f^{28-q-m} \ 5s^{m-1} \ nl + h\nu$

$\rightarrow 4d^{10} \ 4f^{28-q-m+1} \ 5s^{m-1} + h\nu$

$\rightarrow 4d^{10} \ 4f^{28-q-m+1} \ 5s^{m-2} \ n'l' + h\nu \quad (n'=5,6, \quad n \leq n')$

$4d^{10} \ 4f^{28-q-m-1} \ 5s^m \ n'l' \rightarrow 4d^{10} \ 4f^{28-q-m-1} \ 5s^m \ nl + h\nu$

$\rightarrow 4d^{10} \ 4f^{28-q-m} \ 5s^m + h\nu$

$\rightarrow 4d^{10} \ 4f^{28-q-m} \ 5s^{m-1} \ n'l' + h\nu$
Equation of Radiative Transfer

Photon Emissivity Coefficient (PEC)

W^{q+} (q=17-27) ground state 4d^{10} 4f^{m} (m=14-1),
Ionization energy (IE): 432.3 eV-885.7 eV

Upper state \quad Lower state

4d^{10} 4f^{m-1} n’l’ \rightarrow 4d^{10} 4f^{m-1} nl + h\nu
\rightarrow 4d^{10} 4f^{m} + h\nu \quad (n’=n=5)

W^{q+} (q=28-37) ground state 4d^{m} (m=10-1),
Ionization energy (IE): 1133.8 eV-1620.2 eV

4d^{m-1} n’l’ \rightarrow 4d^{m-1} nl + h\nu \quad (n’=4,5, n \leq n’)

W^{q+} (q=38-45) ground state 4s^{m} 4p^{46-q-m} (m=0-2),
Ionization energy (IE): 1830.7 eV-2414.2 eV

[4s^{m} 4p^{46-q-m}]^{-1} n’l’ \rightarrow [4s^{m} 4p^{46-q-m}]^{-1} nl + h\nu
\quad (n’=4,5, n \leq n’)

W^{q+} (q=46-48) ground state 3d^{m} (m=10-8),
Ionization energy (IE): 4059.2 eV-4309.4 eV

3d^{m-1} n’l’ \rightarrow 3d^{m-1}nl + h\nu \quad (n’=n=4)
\rightarrow 3d^{m} + h\nu

FAC data vs. ADAS data

Full J-J coupled level resolved scheme \quad Configuration average scheme

For eg. W^{25+}

Total 9+496 levels \quad 1+28 states
**Impurity injection experiment in KSTAR**

**Shot information**
- **#16958**: $B_T = 2.5$ T with NBI power = 2.8 MW
- 2 – 3 mg of 12 μm W powder was injected at around 4.03 sec ($\#$ of W atoms in 1 mg: $\sim 4.6 \times 10^{18}$)
- Tungsten spectra were measured after the injection by compact advanced EUV spectrometer system (CAES).

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Viewing area of EUV spectrometer (vertically $\sim 18$cm)

W in injected in the mid-plane by injector mounted 10 cm away from LCFS

**#16958 Visible camera images**

On the courtesy of In Woo Song in KAIST and KSTAR team
Measured spectra in KSTAR

- Lines of sight, Thomson $T_e$ & $n_e$ profiles

LoS for CAES on KSTAR

- Simple 2-D configuration (only the pinhole position and the detector position are considered)
- 10 lines of sight (corresponding to 10 channels during #16958)
- Sample points are generated on the LoS with equal distance apart

- Thomson data at 4.15 s (100 ms averaged) are used
- Fitted by using tanh function

On the courtesy of In Woo Song in KAIST and KSTAR team
Measured vs. modeled spectra
Transport free modeled spectra

Fractional abundance from ADAS ca09_w.dat (ionization) and acd50_w.dat (recombination). PEC from FAC calculations.
ADAS ionization data by CADW ab-initio calculation for W ions is reliable within 30-50% accuracy being compared with other ab-initio calculations and the data set is available for all ionization stages.
Recombination data for W
Equation of Radiative Transfer

DR data for W

ABSA recombination data based on a simple Burgess formula for W ions quite differ from other ab-initio calculations and the data is not available for many ionization stages.

IAEA&KAERI Joint CM on DR for W (Sept. 2015)

\[ \alpha_i (T) = \frac{1}{2g_i} \left( \frac{4\pi a_0^2 \text{Ry}}{k_B T} \right)^{3/2} \times \sum_j g_j A_{ji} B_j \exp \left( -\frac{E_{ij}}{k_B T} \right) \times \sum_f \frac{A_{rf}}{A_{jk}} B_f \]

Burgess formula

\[ \alpha_i (T) = 7.59 \times 10^{-14} n_e n_Z \frac{B(q)D(q, T)}{T^{3/2}} \times \sum_j f_{ji} A(y) \exp \left( -\frac{E}{T} \right) \]
IAEA-KAERI joint CM on DR for W

At KAERI (Sept. 2015)
New recommended DR data for W ions

ADNDT in press, available online 5 June 2017
New recommended DR data for W ions

ADNDT in press, available online 5 June 2017
Equation of Radiative Transfer

DR data for W ions (Our calculations)


Equation of Radiative Transfer

DR data for W ions (Our calculations)
Threshold energy of resonance for DR of $W^{q+}$ ($q = 5-11$)

<table>
<thead>
<tr>
<th>Ion</th>
<th>Ground configuration</th>
<th>FAC (eV)</th>
<th>NIST (eV)</th>
<th>% Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>$W^{4+}$</td>
<td>$4f^{14}5s^25p^65d^2$</td>
<td>51.62</td>
<td>51.6</td>
<td>0.04</td>
</tr>
<tr>
<td>$W^{5+}$</td>
<td>$4f^{14}5s^25p^65d$</td>
<td>65.20</td>
<td>64.77</td>
<td>0.66</td>
</tr>
<tr>
<td>$W^{6+}$</td>
<td>$4f^{14}5s^25p^6$</td>
<td>116.92</td>
<td>122.01</td>
<td>4.17</td>
</tr>
<tr>
<td>$W^{7+}$</td>
<td>$4f^{14}5s^25p^5$ or $4f^{13}5s^25p^6$</td>
<td>140.53</td>
<td>141.2</td>
<td>0.47</td>
</tr>
<tr>
<td>$W^{8+}$</td>
<td>$4f^{14}5s^25p^4$</td>
<td>162.17</td>
<td>160.2</td>
<td>1.35</td>
</tr>
<tr>
<td>$W^{9+}$</td>
<td>$4f^{14}5s^25p^3$</td>
<td>180.9</td>
<td>179.0</td>
<td>1.06</td>
</tr>
<tr>
<td>$W^{10+}$</td>
<td>$4f^{14}5s^25p^2$</td>
<td>203.93</td>
<td>208.9</td>
<td>2.38</td>
</tr>
<tr>
<td>$W^{11+}$</td>
<td>$4f^{14}5s^25p$ or $4f^{13}5s^25p^2$</td>
<td>231.6</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Equation of Radiative Transfer

DR data for W ions (Our calculations)

\[ 4f^{14}5s^25p^65d \]
Ground level

\[ 4f^{14}5s^25p^6 \]
Ground level
Equation of Radiative Transfer

DR data for W ions (Our calculations)

$4f^{14}5s^25p^5$
Ground level

$4f^{14}5s^25p^4$
Ground level
DR data for W ions (Our calculations)

4f^{14}5s^25p^3
Ground level

4f^{14}5s^25p^2
Ground level

To be submitted.
Due to so many resonances of $4f$ core excitation, DR via $4f$ transition has been still run.
Spectroscopy in CCP device

Experimental setup

Optical Emission Spectroscopy

13.56 MHz RF CCP

Langmuir Probe
Langmuir probe diagnostics and OES

\[ T_e = 2.6 \text{ eV} \]
\[ n_i = 5.6 \times 10^{15} \text{ m}^{-3} \]

EEPFl: measured by Impedans Ltd. Langmuir probe
Equation of Radiative Transfer

\[ \sum_{j=0}^{4} \alpha_{j1} N_j n_e + \sum_{m=5}^{13} A_{m1} N_m + \sum_{m=5}^{14} \alpha_{m1} N_m n_e \]

\[ \left[ \left( \alpha_{1i} + \sum_{k=0}^{14} \alpha_{1k} \right) n_e + \tau_1^{-1} + \sum_{j=1}^{4} \alpha_{1j} N_j \right] N_1 \]

\[ \sum_{j=0}^{4} \alpha_{j2} N_j n_e + \sum_{m=5}^{14} A_{m2} N_m \]

\[ \left[ \left( \alpha_{2i} + \sum_{k=0}^{4} \alpha_{2k} \right) n_e + A_{2}^{\text{eff}} + \sum_{j=1}^{4} \alpha_{2j} N_j \right] N_2 \]

\[ \sum_{j=0}^{4} \alpha_{j3} N_j n_e + \sum_{m=5}^{14} A_{m3} N_m + \sum_{m=5}^{14} \alpha_{m3} N_m n_e \]

\[ \left[ \left( \alpha_{3i} + \sum_{k=0}^{14} \alpha_{3k} \right) n_e + \tau_3^{-1} + \sum_{j=1}^{4} \alpha_{3j} N_j \right] N_3 \]

\[ \sum_{j=0}^{4} \alpha_{j4} N_j n_e + \sum_{m=5}^{14} A_{m4} N_m \]

\[ \left[ \left( \alpha_{4i} + \sum_{k=0}^{3} \alpha_{4k} \right) n_e + A_{4}^{\text{eff}} + \sum_{j=1}^{4} \alpha_{4j} N_j \right] N_4 \]

\[ \sum_{j=0,1,3} \alpha_{jm} N_j n_e = \sum_{k=m}^{A_{mk}} A_{mk}^{(\text{eff})} N_m + \left( \alpha_{mi} + \sum_{k=0,1,3} \alpha_{mk} \right) N_m n_e \]

\[ N_0 : \text{Ground state } 3p^6 \, ^1S_0 \]

\[ N_{j=1-4} : \text{Metastable} (j = 1, 3) \text{ and resonance} (j = 2, 4) \text{ states } 1s_{5-2}, \, 3p^5 \, 4s \, ^2S+1P_j \]

\[ N_{m=5-14} : \text{Excited states} 2p_{10-1} , \, 3p^5 \, 4p \, ^2S+1L_j \]

Under construction!
Database updates

Our website for atomic data and CR modeling

http://pearl.kaeri.re.kr
1. We have calculated PEC for tungsten (W) ions $W^{q+}$ ($q = 5-48$) by parallelizing radiative transition routine of FAC.

2. We had compiled available DR data for W ions and gave the recommended data through IAEA and KAERI joint CM.

3. We have calculated DR for $W^{q+}$ ($q = 5-11, 44-46$) and will calculate DR for $W^{q+}$ ($q = 30-34$).

4. We have installed a CCP device and measured plasma temperature and density for Ar with a Langmoir probe. OES for Ar has also been carried out. CR modeling including detailed collision and radiative processes will be constructed.

5. We have updated the calculated atomic data and implemented the previous CR modeling for He I on our Web DB (http://pearl.kaeri.re.kr).

6. Parallelization for FAC was done for AI routine will be performed.

7. Unitary correction for collisional excitation routine based on distorted wave approximation of FAC will be tried.
Collaborations

Dept. of Physics, Fusion Plasma Transport Research Center

ITER Korea VUV Diagnostic Team, KSTAR Team

Physical Metrology team: Absolute calibration for spectrometer
Fractional abundance

\[ N_{\text{tot}} = \sum_{i=0}^{Z} N^i, \quad f^q = \frac{N^q}{N_{\text{tot}}} \]

Fractional Abundance

\[ \sum_{i=0}^{Z} f^i = 1. \]

Collisional Ionization Equilibrium

Total recombination rate coefficient

\[ N_{\text{tot}} \frac{d}{dt} \begin{bmatrix} f^0 \\ f^1 \\ \vdots \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \end{bmatrix} \]

Total ionization rate coefficient

\[ N_{\text{tot}} n_e \begin{bmatrix} -S_{\text{tot}}^{0\to 1} \\ S_{\text{tot}}^{0\to 1} - \alpha_{\text{tot}}^{1\to 0} - S_{\text{tot}}^{1\to 2} \alpha_{\text{tot}}^{2\to 1} \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} f^0 \\ f^1 \\ \vdots \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \]
W VUV Spectra measured in KSTAR

Electron temperature

Electron density

KSTAR #13104
(Before) 5.205
(After) 5.405 5.511 5.711

Main ions emitting 14-25 nm VUV

Transport free spectrum

- Post-processing
  1. Neutron noise subtraction
  2. Time average (~40 ms, 3 frames)
Fractional abundance difference

Electron temperature (eV)
Spectra sensitivity

![Graph showing spectra sensitivity with two curves labeled ADAS FA and New FA. The graph plots emissivity against wavelength (nm). The peaks at W⁵⁺ - W⁴⁺ are highlighted.]
Modeling uncertainties

- Electron temperature & density profiles
- Transport D & V coefficients
- Time evolution of impurity
- Atomic data for ionization and recombination
- PEC beyond coronal model